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                 alerts (SDIs) affected
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                CERAB reloaded; updating to resume; current-awareness
      12 DEC 17
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     13 DEC 17
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NEWS 15 DEC 30
                No connect-hour charges in EPFULL during January and
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     19 FEB 16
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NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

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FILE LAST UPDATED: 19 FEB 2005 (20050219/UP). FILE COVERS 1950 TO DATE.

On December 19, 2004, the 2005 MeSH terms were loaded.

Warning: The search L-number/HUMAN limit is missing from records indexed with the new 2005 MeSH (records added since December 19, 2004). Until this is corrected, include HUMANS/CT and 20041219-20051231/ED in searches to limit results to humans for this time period.

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MEDLINE thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2005 vocabulary. See http://www.nlm.nih.gov/mesh/ and http://www.nlm.nih.gov/pubs/techbull/nd03/nd03\_mesh.html for a description of changes.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s combinatorial (w) library

6963 COMBINATORIAL

56752 LIBRARY

L1 578 COMBINATORIAL (W) LIBRARY

=> s l1 and cluster

48241 CLUSTER

L2 6 L1 AND CLUSTER

=> s 12 and rms

3143 RMS

L3 0 L2 AND RMS

=> FIL MEDLINE CAPLUS

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FILE 'CAPLUS' ENTERED AT 14:18:11 ON 22 FEB 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

=> s combinatorial (w) library

L4 7965 COMBINATORIAL (W) LIBRARY

=> s 14 and cluster

L5 62 L4 AND CLUSTER

=> s 15 and rms

L6 1 L5 AND RMS

=> d 16 ab

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN L6 In a computational method of assessing a combinatorial AB library for complementarity to a target mol., ligands from the library are first docked to the target mol. The docking results are clustered using as a metric the rms deviation between the core of two docked mols. The library is rated as to complementarity to the target mol. according to the relative number of ligands in the top cluster. => d 16 1 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN L6 2002:158328 CAPLUS AN136:194220 DN Prioritization of combinatorial library screening TΙ Diller, David J.; Merz, Kenneth M. IN PA U.S. Pat. Appl. Publ., 25 pp., Cont.-in-part of U.S. Ser. No. 595,096. SO CODEN: USXXCO ידת Patent English LA FAN.CNT 1 APPLICATION NO. DATE KIND DATE PATENT NO. \_\_\_\_\_ \_\_\_\_\_\_ ----\_\_\_\_\_ 20020228 US 2001-832786 20010411 US 2002025535 Α1 PΙ WO 2001-US19318 20010615 WO 2001097098 A2 20011220 WO 2001097098 **A3** 20030828 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG 20031211 US 2002-320752 20021216 US 2003228624 Α1 PRAI US 2000-595096 A2 20000615 20010411 US 2001-832786 Α 20010615 WO 2001-US19318 Α1 => s library 126865 LIBRARY L7 => s 17 and cluster 2662 L7 AND CLUSTER => s 18 and rms L9 1 L8 AND RMS => d 19 ab ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN 1.9 In a computational method of assessing a combinatorial library for complementarity to a target mol., ligands from the library are first docked to the target mol. The docking results are clustered using as a metric the rms deviation between the core of two docked mols. The library is rated as to complementarity to the target mol. according to the relative number of ligands in the top

cluster.